

COMBUSTION AND FLOW MODELLING APPLIED TO THE OMV VTE⁺Louis M. Larosiliere^{*} and San-Mou Jeng^{**}

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ABSTRACT

A predictive tool for hypergolic bipropellant spray combustion and flow evolution in the OMV VTE is described. It encompasses a computational technique for the gas phase governing equations, a discrete particle method for liquid bipropellant sprays, and constitutive models for combustion chemistry, interphase exchanges, and unlike impinging liquid hypergolic stream interactions. Emphasis is placed on the phenomenological modelling of the hypergolic liquid bipropellant gasification processes. An application to the OMV VTE combustion chamber is given in order to show some of the capabilities and inadequacies of this tool.

Introduction

Small rocket engines are typically employed in propulsion applications requiring relatively low thrust levels and total impulse. An example of such applications is attitude control systems for vehicle orientation and orbital or plane maneuvers. TRW is currently developing a hypergolic bipropellant variable thrust engine (VTE) to be qualified specifically for the orbital maneuvering vehicle (OMV). The available analytical prediction methodology is incapable of providing physical and phenomenological insight about the complex spray combustion and flow processes occurring within thrust chambers such as the VTE. Thus, an evolutionary prediction methodology that is comprehensive enough to allow

local resolution of certain observable critical processes is needed. The work to be described herein is stimulated by the desire to model some of the critical processes within a hypergolic bipropellant thruster.

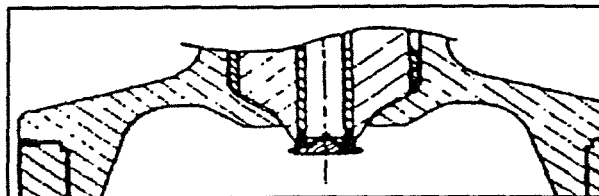


Figure 1. Small rocket thruster configuration.

Thrust chambers involving hypergolic liquid bipropellants reveal a multitude of complex chemical and physical phenomena. These phenomena include homogeneous and heterogeneous chemical reactions, liquid phase dynamics, and turbulent gas transport. A typical thrust chamber of interest is sketched in Figure 1. Injection of a hypergolic bipropellant system is accomplished via a single element coaxial flow injector with a throttling sleeve. One propellant stream flows as an axially directed jet while the other stream is turned radially just prior to injection. A complete description of the ensuing developments soon after injection is not available. It is believed that the jets impinge forming oxidizer and fuel sheets in the immediate vicinity of the injection ports. Because of the hypergolicity of the bipropellant system, chemical reactions and heat release during impingement may result in ignition within the sheets and, hence, affect the atomization, mixing and combustion of the propellants. Subsequently, the sheets disintegrate into ligaments and these ligaments eventually form a spray containing a wide spectrum of attributes. Thereafter, liquid spray droplet aerothermodynamics along with the turbulent gas transport dominate.

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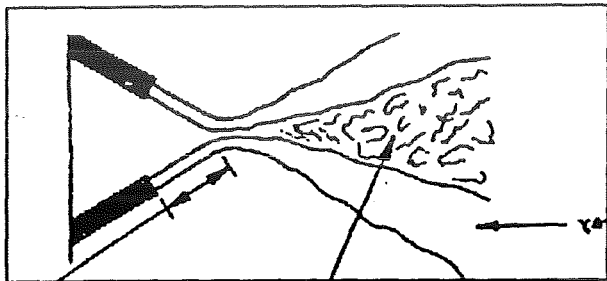


Figure 2. Hypergolic stream separation.

Previous applied research work and investigative studies have shown that a wide range of coupled and interrelated processes are manifested in a hypergolic bipropellant thruster. Elverum and Staudhammer¹ first reported that impinging hypergolic liquid streams under certain conditions have a tendency to be blown apart rather than achieve the intended degree of mixing. Burrows² and Breen et al³ have made photographic observations of the impingement of two hypergolic liquid streams confirming this hypergolic stream separation tendency. Tentative criteria to predict the presence or absence of hypergolic stream separation have been advanced by Kushida and Houseman⁴ on the basis of theoretical analysis. Their results showed that depending on the pressure level, stream separation originated from either liquid/liquid interfacial reactions or gas phase reactions. The physical nature of the separation process, when it did occur, was generally presumed to involve a quasi-steady lamination of the spray fans with fuel on one side and oxidizer on the other (Figure 2). Campbell et al⁵ demonstrated by way of photography that the hypergolic stream separation phenomenon is a cyclic process in which explosions disrupt the spray fan and drive the jets apart, thereby producing temporary physical separation of fuel and oxidizer.

Somogyi and Feiler⁶ determined the heat release rates produced by the reactions of hydrazine with nitric acid in a bomb calorimeter under conditions of forced mixing. Its heat release depends on the interfacial area between the propellants. A combustion mechanism based on bipropellant interfacial reaction was postulated for highly reactive bipropellant systems under conditions of forced mixing. This interfacial reaction process along with the usual liquid droplet combustion mechanisms emerge as the most likely modes of propellant gasification within a hypergolic thruster. Attempts at quantifying the relative importance of these two

gasification modes have either not been successful or were not reported.

Most current models⁷ for performance analysis of rocket combustion tend to decouple the critical processes. A zonal approach is usually taken whereby different assumed physical processes of interest are modeled and then conveniently connected. Liang et al⁸ constructed a computational model for the rocket combustion of H₂/LOX with coaxial injection. They described a comprehensive three-phase (liquid, gas, and spray droplets) model capable of resolving some of the atomization length and time scales. This model is computationally too intensive and not directly applicable to a liquid hypergolic bipropellant system. The state-of-the art in spray combustion modelling requires as external input an ample amount of injection system characterization in order to be useful. Recent developments⁹ in spray combustion modelling aimed at the gas turbine and internal combustion engine arena have produced a wealth of simulation techniques which haven't yet been fully applied to the rocket engine combustor. Creative exploitation of these techniques for the case of a hypergolic bipropellant system remains to be done.

This paper discusses a fundamental CFD-based modelling approach which is under development for analyzing the hypergolic bipropellant spray combustion and flow evolution in the VTE thruster. An inclusive physical model is formulated and integrated within the computational framework of the KIVA-II¹⁰ chemically reactive flow code developed for internal combustion engines. Emphasis is placed on the "sub-scale" modelling of the hypergolic liquid bipropellant gasification processes. The model is applied to the VTE thrust chamber configuration employing the bipropellant system of N₂H₄/N₂O₄. Some of the more doubtful elements of the model are identified for further refinements.

Model Formulation

Consider the thrust chamber to be a closed volume containing a reactive gas and allow a pair of continuous liquid phases to be introduced into it via an injection system. Upon entering the volume, the two distinct liquid phases will undergo mutual interactions as well as interactions with the gas phase. A tendency to disintegrate will set in and eventually the liquid will breakup into ligaments and a spectrum of different drop sizes, and through different intermediate steps, depending on the relative

magnitudes of the aerodynamic, viscous, inertia and surface forces at play. Concurrently, the motion of the gas is altered by the interfacial exchanges with the liquid. Hence, the realm of two-phase flow is entered. Although conservation equations may be formulated for both phases, it should be noted that for the liquid phases, physical conservation only has meaning over a finite portion of the volume and a finite time interval. This is due to the discontinuous breakup and turbulent dispersion processes. In order to keep the problem manageable, a model consisting of two dispersed liquid phases imbedded within a continuum gas is formulated. The dispersed liquid phases are taken to be collections of quasi-spherical liquid material volumes (i.e. "globules") capable of undergoing deformations and breakup. Details of the derivations may be found by consulting the dissertation of O'Rourke¹¹. A brief description of the mathematical model follows.

Dispersed Liquid Phase

The evolution in space and time of certain average properties of a collection of entities may be obtained in a manner analogous to the method of kinetic theory. A globule number distribution function is defined for globules of composition j in such a way that

$$f_j(\vec{S}_j, t) dV_j \quad j=1, 2$$

is the probable average number of globules in the infinitesimal globule hyper volume. The subscript j differentiates between oxidizer and fuel globules. \vec{S}_j is a vector whose coordinates give the values of those properties specifying the state of a globule at a given instant.

$$dV_j = ds_{j_1} ds_{j_2} \dots ds_{j_N}$$

is the infinitesimal globule hyper volume in the N dimensional state space. A stochastic equation giving the rate of change of the distribution function over a continuous time interval follows:

$$\begin{aligned} \frac{d_j}{dt} \int f(\vec{S}_j, t) dV_j = & \int \dot{f}_{coll,j} dV_j \\ & + \int \dot{f}_{bu,j} dV_j \end{aligned} \quad (1)$$

This equation states that the rate of change of globule number along the globule trajectory in its state space is balanced by: collision rates among globules of the

same composition as well as those of another composition, and breakup rates. The globule state vector is taken to be:

$$\vec{S}_j = \begin{bmatrix} \vec{x}_j \\ \vec{v}_j \\ r_j \\ T_{d,j} \\ y_j \\ \dot{y}_j \end{bmatrix}$$

where,

\vec{x}_j globule position vector,
 \vec{v}_j globule velocity vector,
 r_j globule radius,
 $T_{d,j}$ globule temperature,
 y_j globule spherical deviation,
 \dot{y}_j globule oscillation.

The evolution equations for the globule state variables may be obtained by taking appropriate moments of equation (1). Characteristic equations governing the trajectory, acceleration, vaporization, heat-up, deformation, and oscillation of a globule are thus furnished. These are Lagrangian equations describing the development of the state of a globule from some initial state.

Continuum Gas Phase

Equation (1) is directly coupled with the gas dynamics. The Navier-Stokes equations are valid for the average gas properties provided suitable source terms are added to account for the effect of the dispersed liquid phases. In the formulation, the averaging is carried over the entire spatial volume. Hence, the gas properties are viewed as being continuously distributed throughout the entire volume. This point of view eliminates the need to carry along the direct effect of the liquid phase volume displacement. If the gas is considered to be a turbulent reactive mixture of ideal gases, equations for the conservation of species mass, mixture momentum, and internal energy may be formulated. A modified k-epsilon turbulence closure along with a gradient diffusion model are employed to describe the fluctuation correlations. When the source terms are given along with initial and boundary conditions, a solution may be sought describing the average gas field variables.

The limitations of the present formulation are the source term modelling, and the numerical solution technique. These two subjects are considered next.

Sub-Scale Modelling

Sub-scale modelling attempts to describe phenomena occurring on a scale much smaller than that of the macroscale view. The formulation needs a certain degree of a priori knowledge of phenomenological processes occurring on the sub-scale level. As such, it lacks the details and also the fidelity of the macroscale model.

Dispersed Phase Interactions

The collision source term in equation (1) depends upon the details of globule interactions. Only binary collisions are considered. Following the analysis of Williams¹² under the assumption that globule collisions are similar to collisions among hard spheres, an expression may be formulated for the collision source term. The derivation is complex and will not be repeated here. Suffice to say that the result is:

$$\dot{F}_{coll, \alpha} = \Gamma_{\alpha}^{(+)} - \Gamma_{\alpha}^{(-)}$$

where,

$$\begin{aligned} \Gamma_{\alpha}^{(-)} = & \int f_{\alpha}(\xi'_{\alpha}, \bar{x}, t) |\bar{v}'_{\alpha} - \bar{v}_{\alpha}| \sigma^{(-)}(\xi_{\alpha}; \xi'_{\alpha}) d\xi'_{\alpha} \\ & + \int f_{\alpha}(\xi_{\alpha}, \bar{x}, t) |\bar{v}_{\alpha} - \bar{v}_{\beta}| \sigma^{(-)}(\xi_{\alpha}; \xi_{\beta}) d\xi_{\beta} \end{aligned}$$

$$\begin{aligned} \Gamma_{\alpha}^{(+)} = & \int f_{\alpha}(\xi'_{\alpha}, \bar{x}, t) f_{\alpha}(\xi''_{\alpha}, \bar{x}, t) |\bar{v}'_{\alpha} - \bar{v}''_{\alpha}| \sigma^{(+)} d\xi'_{\alpha} d\xi''_{\alpha} \\ & + \int f_{\alpha}(\xi_{\alpha}, \bar{x}, t) f_{\beta}(\xi_{\beta}, \bar{x}, t) |\bar{v}_{\alpha} - \bar{v}_{\beta}| \sigma^{(+)} d\xi_{\alpha} d\xi_{\beta} \end{aligned}$$

$$\xi = \begin{bmatrix} \bar{v} \\ x \\ y \\ \bar{T} \\ d \end{bmatrix}$$

The above expressions include both the effects of collisions among globules of the same composition as well as those among α and β globules. Provided aerodynamic distortions of the globules are small, an expression for the geometrical collision crosssection is:

$$\sigma^{(+)}(\xi; \xi') = \pi (x + x')^2$$

The differential crosssection for the production of globules, $\sigma^{(+)}$ needs to be modelled depending on the outcomes of a collision.

Collisions among globules of the same composition are rare under the present circumstances and will not be discussed further. The possible outcomes of a collision between alpha and beta globules are postulated to be: 1) an interface contact collision whereby the globules maintain their sizes and temperatures but undergo velocity changes, or 2) an interfacial mixing allowing for the possibility of an interfacial chemical reaction. The boundaries of these two possible outcomes are defined by a reaction probability function given by:

$$\eta_c = \frac{\tau_{res}}{\tau_{chem}}$$

where the interfacial residence time under the assumption that the alpha globule is the larger of the two is,

$$\tau_{res} = \frac{1}{\int \pi (x_{\beta} + x_{\alpha})^2 |\bar{v}_{\alpha} - \bar{v}_{\beta}| f_{\beta}(\xi_{\beta}, \bar{x}, t) d\xi_{\beta}}$$

and the chemical conversion time is,

$$\tau_{chem} = \frac{1}{\int k_r(T_1) v_{\beta} \frac{m_{\beta}}{\rho_{\beta}} f_{\beta}(\xi_{\beta}, \bar{x}, t) d\xi_{\beta}}$$

The reaction rate is assumed to have an Arrhenius temperature dependence so that

$$k_r(T_1) = A \exp\left(-\frac{E_a}{T_1}\right)$$

A critical impact parameter is defined as:

$$b_{cx}^2 = \eta_c (x_{\alpha} + x_{\beta})^2$$

If the impact parameter is greater than the critical impact parameter, a non-reacting contact collision is possible otherwise, an interfacial chemical reaction results. When a reaction results, the law of mass action is employed along with a chemical stoichiometry in order to calculate the rate of change of the liquid mass concentration. The globule velocities and temperature are set equal to the liquid temperature and velocity in the volume containing the globules. For a non-reacting contact reaction, the

globule velocities are assumed to be the same as the liquid velocity. The differential crosssection for production of globules may be written as:

$$\sigma^{(c)}(\xi; \xi_a, \xi_b) = \pi \frac{b_{cr}^2}{2} [\delta(\xi - \xi_a^c) - \delta(\xi - \xi_b^c)] \\ + \pi \int_{b_{cr}}^{\xi_a + \xi_b} [\delta(\xi - \xi_a') + \delta(\xi - \xi_b')] d\xi$$

where the superscript c and the prime refer to appropriate values of the state variables after collision.

Dispersed Phase Breakup

The globule breakup model is based upon a spring-mass analogy developed by O'Rourke and Amsden¹³. This model was formulated for a single component spray. Nevertheless, it is being applied separately to either oxidizer or fuel sprays since the two streams are immiscible. Breakup times are adequately predicted for the "bag" and "stripping" breakup regimes. Product drop sizes and distributions are not directly predicted by the model. Energy conservation arguments are invoked in order to derive product drop average sizes which are then distributed via a chi-squared distribution.

Droplet Combustion

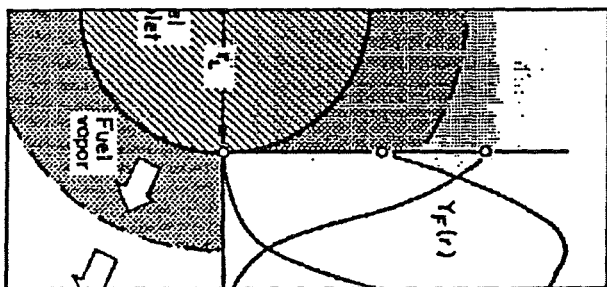


Figure 3. Decomposition flame monopropellant droplet vaporization.

Once the globules breakup into droplets, vaporization becomes dominant. Presently, only isolated droplet vaporization is considered. An extensive review of droplet vaporization has been given by Faeth¹⁴. For high ambient temperatures, experiments reveal the formation of an exothermic decomposition flame enveloping the hydrazine-based fuel droplets as depicted in Figure 3. The existence of the decomposition flame depends on the convective environment and the decomposition kinetics. Two modes of vaporization are considered for the fuel

droplet vaporization: 1) decomposition flame within a diffusion mantle, or 2) pure diffusion flame without any decomposition. The formulation of the model is an adaptation of that given by Faeth¹⁵ for pure monopropellant droplets.

Detail computations of the vaporization of N₂O₄ droplets show that an endothermic decomposition occurs rapidly very close to the droplet surface. A bipropellant droplet vaporization model given in reference 14 has been used by many other investigators for the N₂O₄ droplets. For lack of a better model, the same procedure is invoked here.

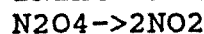
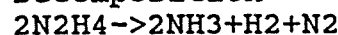
Gas Phase Chemistry

The N₂H₄-N₂O₄ chemistry has been investigated by Sawyer¹⁶. It was surmised that the N₂H₄-N₂O₄ reaction is a two step process. The initial step is the reduction of the NO₂ formed from N₂O₄ decomposition to NO by the action of hydrazine. The second step is the decomposition of hydrazine and the reduction of NO. A five step chemical kinetic scheme (Table I) is employed herein. Equilibrium reactions are not considered since the kinetic reaction rates for this hypergolic system are sufficiently fast to allow the flame-front to propagate.

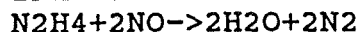
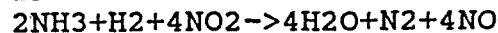
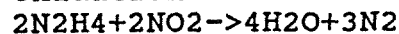
Table I Gas phase kinetic reactions.

N₂H₄-N₂O₄ System:

Decomposition



Oxidation



Droplet Acceleration and Turbulence Dispersion

The acceleration of a droplet depends on the external forces exerted upon it. For the present application, only skin friction and separation drag are considered. Correlations¹⁷ which allow both for vaporization and distortion are employed for the drag coefficient.

The turbulence effects on droplet motion are simulated stochastically by superimposing upon the gas field turbulent eddies each having a length, lifetime, and fluctuation velocities. A discussion of the technique is given by Faeth¹⁸.

Solution Procedure

The approach to solving the globule number conservation equation is to discretize the globule streams into computational parcels that follow globule characteristic paths. Each parcel represents a number of globules of identical states. In the KIVA-II code, the globule number distribution function is approximated by Dirac delta functions. Representing the globule streams by discrete parcels rather than by continuous distributions amounts to a statistical description of the problem, since the finite number of parcels used represents a sample of the total globule population. The globule characteristic equations are integrated implicitly where appropriate due to their strong coupling with the gas phase. Thus, the dispersed liquid phase solution procedure amounts to what is called a stochastic discrete particle tracking.

The gas phase solution procedure is based on an axisymmetric finite volume method called the ALE (Arbitrary Lagrangian Eulerian) method. A staggered mesh is used wherein scalar quantities are defined at cell centers and velocity components at cell vertices. The momentum equation is integrated over momentum cells centered around each grid nodes. Time marching is performed by use of operator splitting and the solution is advanced in a series of phases. A Lagrangian phase whereby the grid nodes move with the local flow is performed first, followed by a rezone phase to set the required grid motion relative to the flow, and finally a convective fluxing phase. Processes that strongly couple the globule and spray dynamics are treated implicitly. A variable implicitness is employed in the gas phase time marching algorithm along with a SIMPLE-styled pressure correction procedure. Details of the computational scheme are fully described in reference 10.

Application to the OMV VTE

The OMV VTE thrust chamber configuration with a central single element coaxial injector is modelled with the N₂H₄-N₂O₄ propellant system. In this simulation, it is assumed that spray droplets are formed right at the injection ports. Hence, the stream impingement and breakup processes are not

Table II Conditions for spray combustion simulation.

	N ₂ H ₄	N ₂ O ₄
SMD (cm)	4.E-3	5.2E-3
Cone ang.	20.0	20.0
Tilt ang.	40.0	40.0
V _{inj} (cm/s)	1270.	1300.
T _{inj} (K)	320.	310.

modelled. This case is a baseline case of pure spray combustion with some details of the injection system characteristics known. Table II lists the relevant parameters for this simulation.

At time zero, N₂H₄ and N₂O₄ spray droplets with a Sauter Mean Diameter (SMD) as given in an Table II are introduced within a volume containing an initially inert gas (N₂). A chi-squared initial drop size distribution is used. The spray droplets interact only with the gas via momentum, mass, energy, and turbulence exchanges. Liquid droplet vaporization is the only gasification mode for this simulation. The computational grid is illustrated in Figure 4. Since this is an axisymmetric configuration, only half of the geometry is discretized. After a time of about 4 ms, an almost steady state combustion is established. Figures 5 and 6 show the droplet trajectories at this time. It may be observed that both fuel and oxidizer droplets are found near the wall especially near the cylindrical portion. The wall boundary conditions are set as free-slip with wall velocities determined by a wall function matching approach. An adiabatic wall temperature is specified along with a constant pressure outflow boundary condition. The propellant mass flow rate is 197 grams/s with an oxidizer fuel ratio of 1.25. Spray injection is accomplished by injecting 100000 parcels per second in such a way as to establish the required propellant mass flow rate. Figure 7 shows the axisymmetric velocity field at a time of 4 ms. A small recirculation region is established in the injector bowl close to the injector face. The average velocity inside the chamber is about 30 m/s. Away from the injector, a unidirectional flow field prevails. The pressure temperature fields are illustrated in Figure 8. A maximum temperature of 2200 K along with an

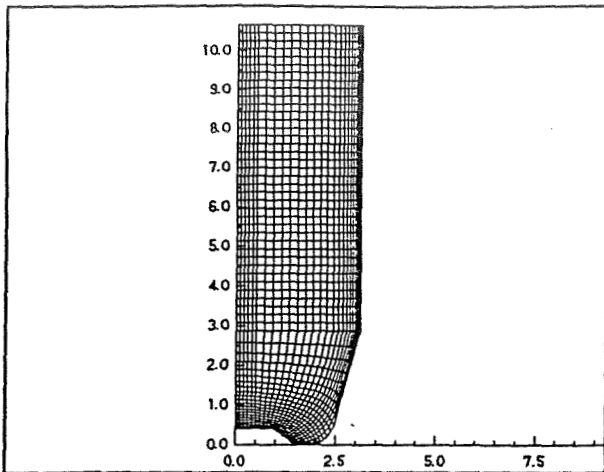


Figure 4. OMV VTE thrust chamber computational grid.



Figure 5. N₂H₄ spray droplet velocity field.



Figure 6. N₂O₄ spray droplet velocity field.

average pressure of about 7 atm can be seen within the chamber. Mass fraction contours are presented in Figure 9. Propellant decomposition is marked by regions of NH₃ for hydrazine and NO₂ for nitrogen tetroxide. It may be noted that a majority of the hydrazine decomposition occurs near the chamber axis where the relative velocity between the gas and a droplet is low.

Summary and Conclusions

An inclusive modelling framework has been established for the VTE thrust chamber. The gross effects of the injection and atomization processes are included. Computational and experimental tests are required to fine tune some of the sub-models. A

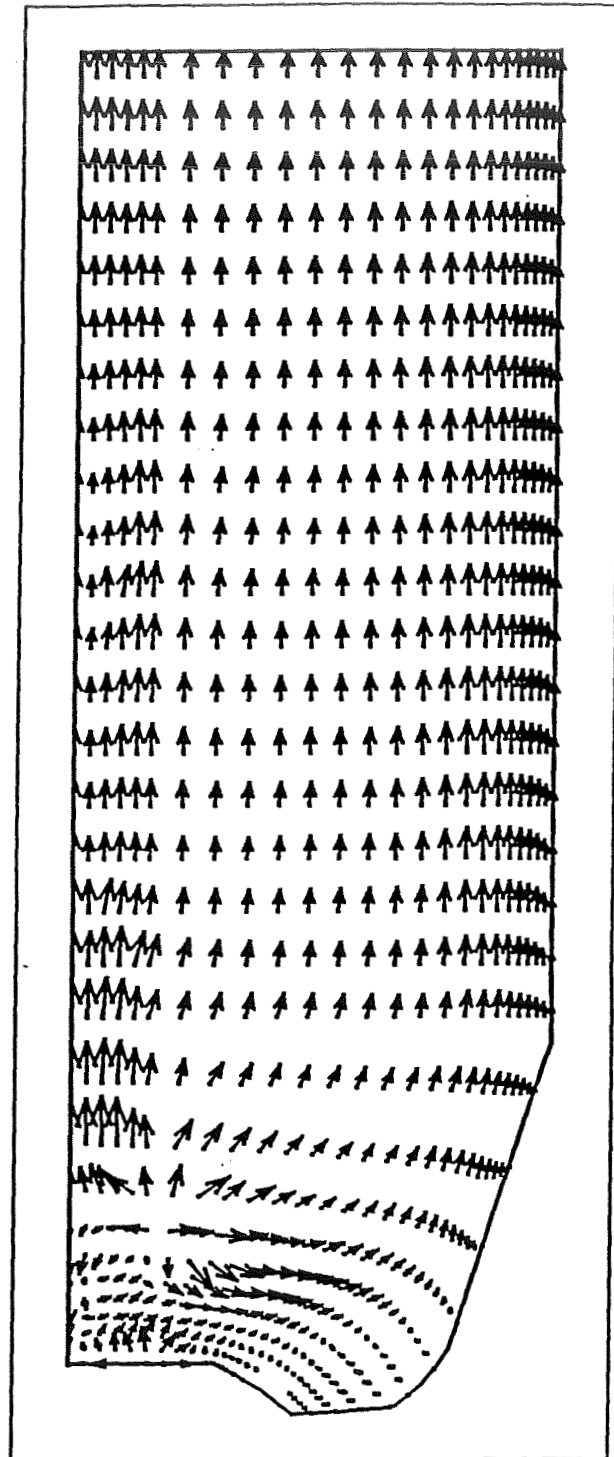


Figure 7. Axisymmetric gas velocity field.

baseline computation of pure spray combustion without the effects of spray interactions has been given. Future computations with the complete model

are forthcoming. After further refinements, this model should prove most useful in the development of small rocket thrusters such as the VTE.

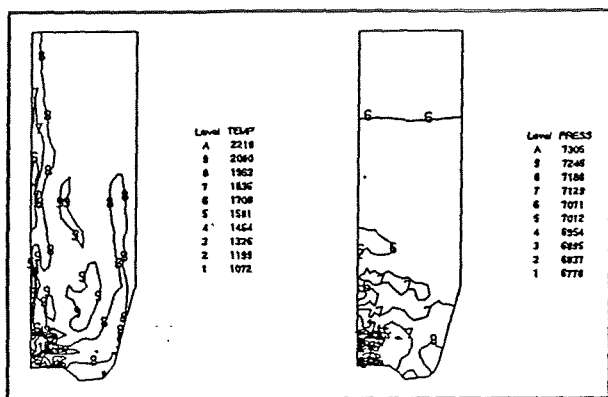


Figure 8. Gas temperature and pressure contours at a time of 4 ms.

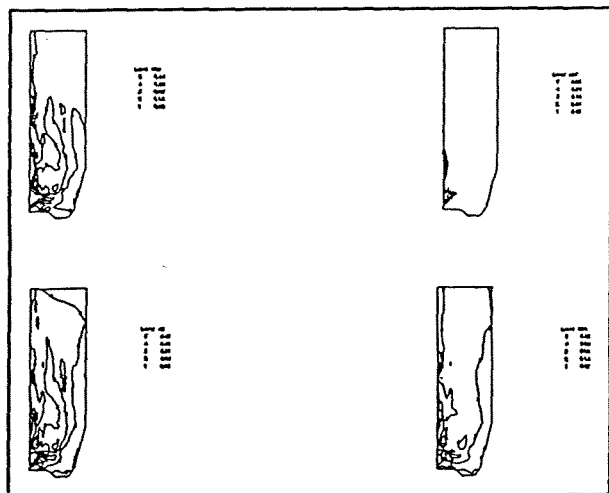


Figure 9. Species mass fraction contours: N₂, H₂O, NH₃, NO₂.

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